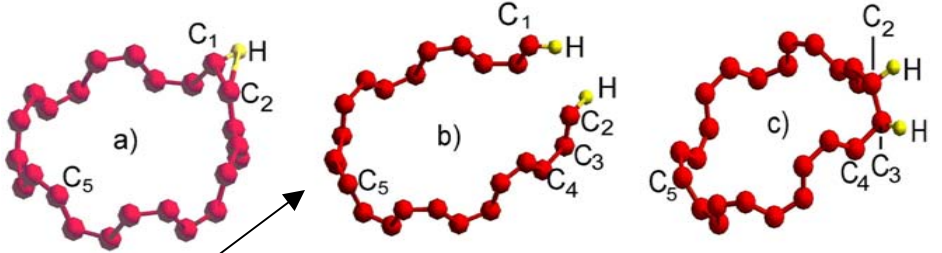


Hydrogen-induced Unzipping of Single-Walled Carbon Nanotubes

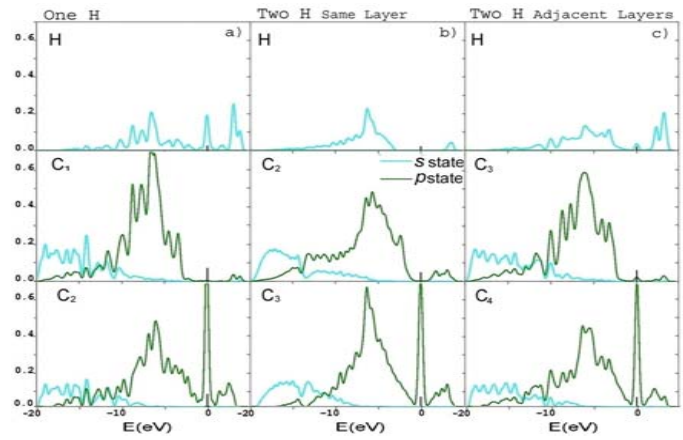
Storage of Hydrogen by Carbon nanotubes has shown great promise and attracted much attention. Recently, Smalley and coworkers discovered a remarkable phenomenon: under atomic H atmosphere, single-walled nanotubes annealed at 1500°C coalesce with neighboring tubes. We have studied the chemisorption of atomic H on the single-walled armchair carbon nanotube with *ab initio* calculations.

A single H atom is found to be chemisorbed on both the inside and outside wall of the nanotube. The binding energy of H adsorption at the exterior of the nanotube is much greater than that at the interior.

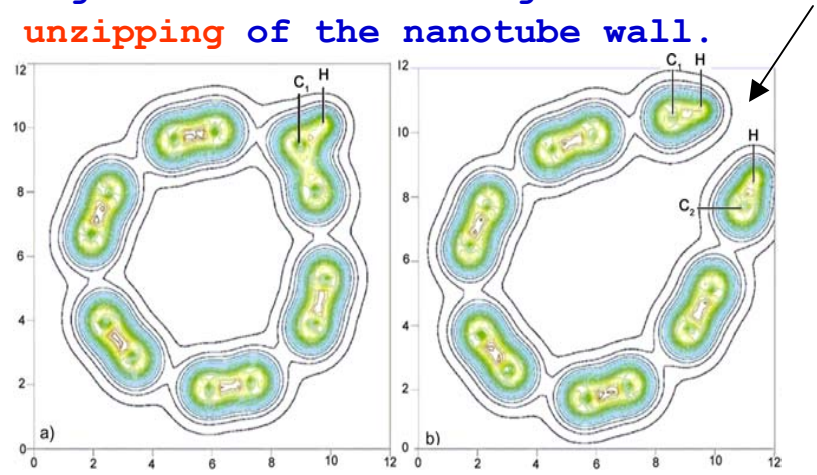
Single H Two H-same layer Two H-adjacent layers



We predict that two rows of H atoms chemisorbed on selective sites exterior to the nanotube can break the nearest-neighbor C-C bond through the concerted formation of C-H bonds, leading to the unzipping of the nanotube wall.



Site and angular momentum Density of states



Charge Density density contour plots

MASSIVELY PARALLEL PLATFORM FOR THE COMPUTATIONAL MATERIALS THEORY CENTER

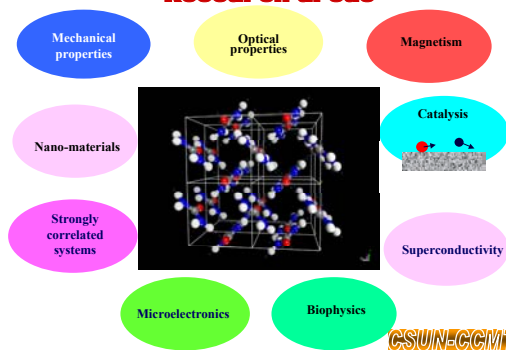
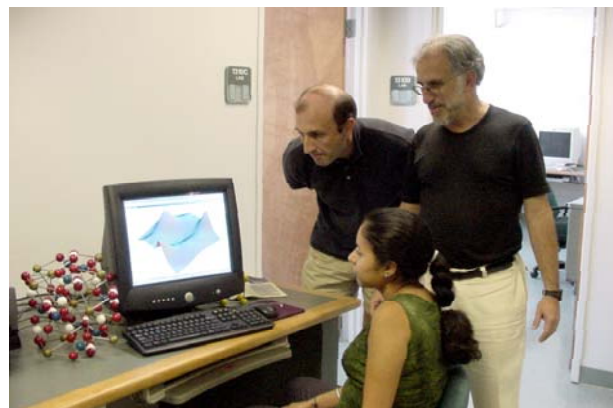
Nicholas Kioussis, D. Sheng, and R. Wu, *California State University Northridge, DMR -00116566*
Education, Outreach and Mentoring

The **Computational Materials Theory Center (CMTC)** includes Profs. N. Kioussis, S.P. Lim, and D. Sheng, postdoctoral fellows, visiting scientists, and graduate/undergraduate students. The **goals** of the CMTC are:

- **To educate and train students** through a program of studies and research activities on future materials-related technological challenges.
- **To conduct fundamental and applied research** that enhances our knowledge in materials properties and processing through theory, modeling, simulation, visualization and computation.
- **To stimulate and develop strong industrial-university-national laboratory** partnerships in materials research.



Research areas



Above: Members of the CMTC:
(Left to right) Front row: T. Sardot, Y. Luo, M. Tovar, and N. Kioussis; Back row: A. Kalitsov, A. Coho, C. Verdozzi, and C. Liu. The 48-CPU SGI2000-3000 and 16-CPU DEC servers in the background.

Above: M. Tovar, C. Verdozzi and N. Kioussis discussing the effect of Hydrogen on the dislocation core properties of Aluminum

Impact on Education

- Hands on Experience on materials related technologies
- Training in coding, parallelization and visualization
- Presentations in professional meetings
- Internships in National/Industrial Laboratories
- Establishment of new interdisciplinary courses in materials science